

Claims

1. A method of analysing a complex hydrocarbon-containing mixture, the method comprising the steps of:
 - obtaining a liquid sample of the complex hydrocarbon-containing mixture;
 - injecting the sample into a liquid carrier flowing to a mass spectrometer, wherein the mass spectrometer is set so as to ionise molecules in the sample without causing fragmentation thereof;
 - recording a first mass spectrum for ions obtained from the sample; and
 - using the mass spectrum to obtain a fingerprint of the mixture.
2. A method as claimed in claim 1, wherein the first mass spectrum is recorded for ions obtained from a first portion of the sample, the method further comprising the steps of:
 - recording one or more further mass spectra for ions obtained from further portions of the sample; and
 - combining the first and further mass spectra to obtain the fingerprint of the mixture.
3. A method as claimed in claim 1 or 2, wherein the sample of the complex hydrocarbon-containing mixture is injected into a continuous flow of eluent fluid to form a plug of the sample within the flow of eluent fluid; and
 - the eluent fluid containing the sample is then supplied to a mass spectrometer for analysis of the sample.
4. A method as claimed in claim 3, wherein the full width half maximum of the concentration of the sample in the eluent over time is determined; and

each of the first and further mass spectra of the sample are recorded by mass spectral analysis of ions generated during the full width half maximum range of the sample.

5. A method as claimed in any preceding claim, wherein the sample is ionised by two or more different ionisation techniques and mass spectra are recorded for the ions obtained by each of the different ionisation techniques.

6. A method as claimed in claim 5, wherein the different ionisation techniques comprise two or more of the following: positive atmospheric pressure electrospray ionisation; negative atmospheric pressure electrospray ionisation; positive atmospheric pressure chemical ionisation; negative atmospheric pressure chemical ionisation; positive atmospheric pressure photoionisation; and negative atmospheric pressure photoionisation.

7. A method as claimed in any preceding claim, wherein:

a plurality of samples are analysed by the method of any preceding claim; and

the mass spectra obtained are analysed using multivariate data analysis.

8. A method as claimed in claim 7, wherein the multivariate analysis used is principal component analysis.

9. A method as claimed in claim 7, wherein the multivariate analysis used is Projections to Latent Structures.

10. A method as claimed in any of claims 2 to 6,

wherein:

the mass spectra obtained for the sample are converted to numerical values;

the numerical values are analysed by principal component analysis; and

the principal components obtained from the analysis of each mass spectrum are plotted to provide a graphical indication of the nature of the sample.

11. A process for monitoring the progress of a reaction comprising the steps of:

taking a sample of the reaction mixture during a reaction;

injecting the sample into a liquid carrier flowing to a mass spectrometer, wherein the mass spectrometer is set so as to ionise molecules in the sample without causing fragmentation thereof;

recording a first mass spectrum for ions obtained from a first portion of the sample;

recording one or more further mass spectra for ions obtained from further portions of the sample;

converting the mass spectra to numerical values;

analysing the numerical values by principal component analysis; and

comparing a plot of the principal components obtained from the analysis of the sample with a plot of the principal components obtained from a sample taken at an earlier stage in the reaction to determine the stage reached by the reaction.

12. A process for controlling a reaction comprising the steps of:

taking a sample of the reaction mixture during a reaction;

injecting the sample into a liquid carrier flowing to a mass spectrometer, wherein the mass spectrometer is

set so as to ionise molecules in the sample without causing fragmentation thereof;

recording a first mass spectrum for ions obtained from a first portion of the sample;

recording one or more further mass spectra for ions obtained from further portions of the sample;

converting the mass spectra to numerical values;

analysing the numerical values by principal component analysis;

comparing a plot of the principal components obtained from the analysis of the sample with the desired position of the principal components for a sample obtained at desirably optimal reaction conditions; and

adjusting the reaction parameters to bring the principal components obtained from the analysis of the sample back towards the desired position.

13. A process as claimed in claim 12, wherein samples are taken and analysed at regular intervals during the reaction and adjustments are made to the reaction parameters in real time in response to the analysis of each sample in order to provide a continuous feedback control process for a reaction.

14. A process for the characterisation of a first complex hydrocarbon-containing mixture, said process comprising:

obtaining a fingerprint of said mixture using a method as claimed in any of claims 1 to 9;

comparing said fingerprint with the fingerprints obtained using a method as claimed in any of claims 1 to 9 of other complex hydrocarbon-containing mixtures of known provenance or properties and thereby determining a prediction of the provenance or properties of said first mixture.